Exploring Infrared Spectroscopy

This experiment explores some features of infrared spectroscopy and introduces you to the use of the technique in identifying unknown compounds.

Organization of the Experiment

Because of the limitations on the infrared spectrophotometer, you will do this experiment in teams of three. Because most of you are in labs with three students on a bench side, this makes a logical team. Each team will have 15-20 minutes to use the spectrophotometer. During that time your lab instructor will demonstrate the infrared spectrometer and run three samples for you. When you are not working in the instrument room, you can be using the computers in the Chemistry Computer Lab to examine spectra and work on identifying your unknown sample as well as describing the important features of several other compounds (Part 4).

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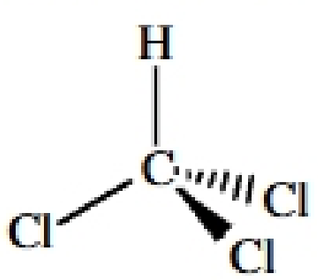
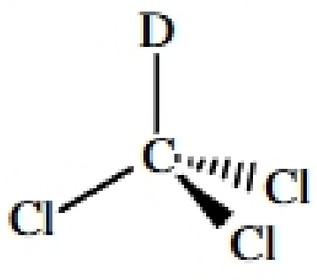
Part 1. Identifying an Unknown

Examine each of the four spectra on pages 3 and 4. On page 1 of the Report Form you will find the structures of four different molecules. Match the molecules and spectra and explain your reasoning in each case.

Part 2. Spectra of $CHCl_3$ and $CDCl_3$



Chloroform



Deuterochloroform

The tetrahedral molecule chloroform, $CHCl_3$, has a C—H bond that has a characteristic stretching vibration around 2900 cm^{-1}. The H can be replaced by a deuterium atom to give $CDCl_3$. Recall that the atomic weight of H is 1.008, whereas a D atom is twice as heavy; it has an atomic weight of 2.014. Your instructor will run the spectrum of one of these compounds for you, and the spectrum of the other will be posted in the instrument room and in the laboratory. Examine these spectra and answer the questions on page 2 of the Report Form.

Part 3. Spectrum of a Packaging Film

Packaging film, the transparent film you use in the kitchen or around the home — Saran wrap, plastic baggies, "cellophane"—is made of organic molecules. Small molecules are joined together to produce polymers, and the polymers are fashioned into various materials such as the polyethylene squeeze bottles we use in the lab.

Each team will bring a piece of packaging film to laboratory and will obtain the infrared spectrum of the film. Spectra of different film will be posted in the instrument room and you will use these to attempt to identify your unknown film. Write up your results on page 3 of the report form.

REMINDER

Each team will bring a small piece of packaging film — 2 inches square — to lab. This can be a piece of a sandwich bag, Saran wrap, or any other transparent film. Be sure to record the source and brandname of your film!

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Part 4. Connecting IR Bands with Vibrations

Note: This portion of the experiment can be done at another time.

One feature of the *Saunders Interactive General Chemistry CD-ROM* is the molecular modeling software. There are hundreds of molecules whose models are in the CAChe folder on the CD. Inside of that folder you will find a folder labeled MODELS and inside of that a folder labeled INFRARED. Inside of that folder are the models of 19 molecules or ions whose spectra have been calculated using the CAChe software (as we have done for SO_2 in *Figure* 2 in the introductory material). To examine a spectrum, proceed as follows:

Note: The calculated IR spectrum on the CD-ROM can only be observed on the Macintosh computers. Use the new iMac computers in the Chemistry Lab.

a) Double click on the icon for a molecule in the INFRARED folder. The file will open in the Visualizer program.

b) When the model appears on the screen, go to the ANALYZE menu and then choose VIBRATIONAL SPECTRA.

c) The vibrational spectrum will appear on the screen. You can deepen and widen the display by holding the mouse key down on the small square at the right hand end of the horizontal axis (just above the 0 marking).

d) The main bands in a spectrum are denoted by small triangles (▲). Click on a triangle, and blue arrows will be superimposed on the model, the arrows showing the movement of atoms in the vibration that gives rise to that band.

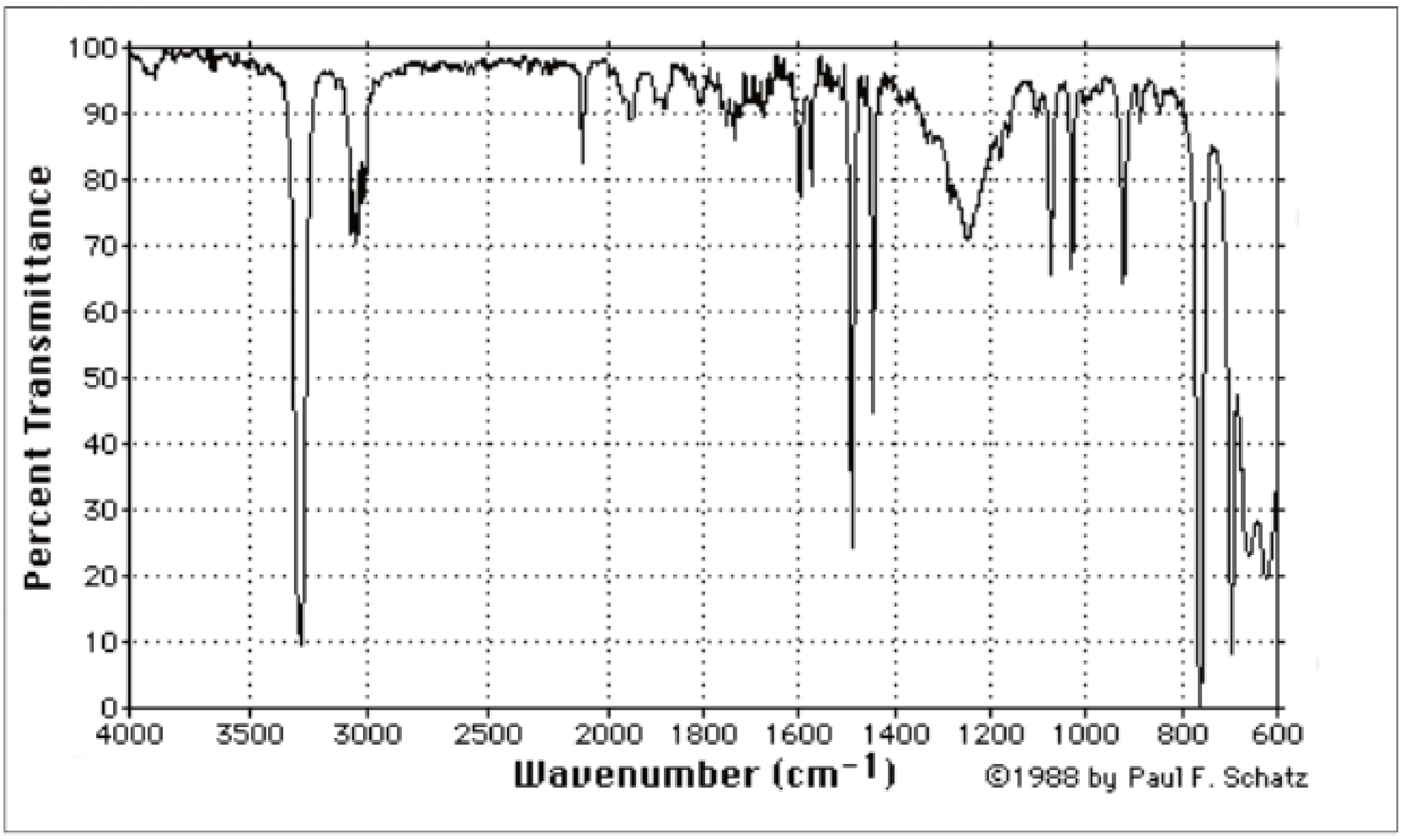
For an illustration of the connection of the spectrum with the vibrations in the molecule see Figure 2 on page 3 of the introductory material.

Part 5. Mystery Compounds

In this portion of the experiment you and your team will run the spectrum of an unknown compound and attempt to identify it. Results are summarized on the Report Form.

Spectra for PART 1 — Identifying an Unknown

Unknown A



Unknown B